

Optimal energy scaling for a shear experiment in single-crystal plasticity with cross-hardening

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Abstract

Consideration is given to a non-convex variational model for a shear experiment in the framework of single-crystal linearised plasticity with infinite cross-hardening. The rectangular shear sample is clamped at each end, and is subjected to a prescribed horizontal or diagonal shear, modelled by an appropriate hard Dirichlet condition. We ask: how much energy is required to impose such a shear, and how does it depend on the aspect ratio? Assuming that just two slip systems are active, we show that there is a critical aspect ratio, above which the energy is strictly positive, and below which it is zero. Furthermore, in the respective regimes determined by the aspect ratio, we prove energy scaling bounds, expressed in terms of the amount of prescribed shear.

1 Introduction and the main model

In this article, we study optimal energy scaling and microstructure formation in the elasto-plastic deformation of single crystals. The main model considered here is a geometrically linear, continuum-mechanical elasto-plastic energy based on the assumption of strong cross-hardening, i.e. that only one slip system can be active at any given point of the material. The basic motivation for our investigation is the following question: can one devise an experiment to determine whether this single-slip condition, taken together with a surface energy which penalises geometrically necessary dislocations (GNDs), is a relevant constraint which needs to be factored into macroscopic models?

The phenomenon of cross- (or latent-) hardening [1, 2, 3] has the effect that activity in one slip system suppresses activity in all other slip systems, which leads to a loss of convexity in the minimization problem associated with the plastic deformation of single crystals [4]. In fatigue experiments, as well as experiments involving only a single-pass deformation, a lamination behaviour is frequently observed [5, 6, 7, 8], and this is believed to stem from cross-hardening [4, 8]. Hence, similarly as in [8], the interest in including cross-hardening in our model, as a side condition on the strain effected by plastic deformation.

The surface energy we include corresponds to the core energy of GNDs. In the geometrically nonlinear setting, the density of the core energy would be of the form $|(\det F^p)^{-1}(\operatorname{curl} F^p)(F^p)^T|$ (see [9, 10, 11] for a discussion), where F^p is the plastic deformation strain, but since we are working in the simpler geometrically linear setting, this leaves us with just the expression $|\operatorname{curl} F^p|$ instead.

Our main results can be described heuristically as follows. We show that the inclusion of both cross-hardening and surface energy significantly affects the energetic scaling in a particular simple shear experiment for single crystals. The experiment modelled is that of a single crystal with a defined orientation of slip systems—realisable, for example, in a B2 crystal structure—and boundary

conditions such that the cuboid crystal is rigidly fixed on its (square) top and bottom faces, according to a prescribed horizontal shear, while remaining free on its four vertical sides. Without either cross hardening or surface energy, the energy infimum in our system is zero (or equal to a certain amount of plastic work if a strain-hardening energy is included) when the aspect ratio of the crystal (base-square side-length/height) is below one, while the energy increases quadratically with the imposed shear magnitude when the aspect ratio is above one. This behaviour changes dramatically when multiple slip is forbidden and GNDs penalised: now the energy only vanishes for aspect ratios smaller than one half, while, again, for aspect ratios above one, the energy grows quadratically with the strain imposed by the boundary conditions. For intermediate aspect ratios, a new regime of linearly growing energy arises. Thus, we conclude that the experiment proposed here can be used to discriminate between those models with surface energy and cross hardening, and those without, and hence to determine whether the inclusion of these effects in macroscopic models for single-pass plastic deformation is physically reasonable.

Kinematically, we restrict ourselves to the case of a cubic crystal structure with $\{011\}\langle 100\rangle$ slip systems. This means that plastic deformation occurs only on planes with normal parallel to one of the three cube axes, and in the direction of one of two Burgers vectors lying diagonally in these planes. Furthermore, we include a surface-energy term consisting of the distributional curl of the plastic deformation, as well as a constant hardening. The domain is a cuboid given by $\Omega_L = (0, 1) \times (0, L) \times (0, 1) \subset \mathbb{R}^3$, and we consider the problem of minimizing the energy

$$E_L(u, \beta) = \int_{\Omega_L} |(\nabla u - \beta)_{\text{sym}}|^2 dx + \sigma \int_{\Omega_L} |\text{curl } \beta| + \tau \int_{\Omega_L} |\beta| dx \quad (1)$$

among vector-valued displacements $u: \Omega_L \rightarrow \mathbb{R}^3$ and matrix-valued plastic deformations $\beta: \Omega_L \rightarrow \mathbb{R}^{3 \times 3}$, for non-negative coefficients σ and τ . Here, the subscript ‘sym’ denotes taking the symmetric part of the matrix in parenthesis. The first term in (1) is the linearized elastic energy of the specimen, and the second term penalizes GNDs, which are quantified by the row-wise curl of the Nye tensor. The third term represents a constant hardening, which for the most part will be neglected by taking $\tau = 0$ (see, however, remark after Thm 3.1).

The admissible displacements for the minimization problem are $u \in H^1(\Omega_L)$, such that $u(\cdot, \cdot, 0) = 0$, $u(\cdot, L, \cdot) = \gamma(1, 0, 0)$ for some parameter $\gamma \geq 0^*$. This models an experiment in which a cuboid specimen with clamped boundary conditions on the top and bottom undergoes a simple shear deformation. Note that the free boundary conditions on the four sides of the specimen are essential in order to render this a physically realisable experiment, and that they also account for most of the technical difficulties in the analysis. While not subject to any boundary conditions, the plastic deformation β must be square integrable, and the absolute value of its distributional row-wise curl should be the density of a finite measure. In the sequel, lower bounds for the energy will be the focus of attention, and all test functions u and β will be (at least piecewise) smooth—this does not represent a further restriction, since any admissible deformation can be approximated in energy by a smooth one.

The single-slip condition translates into a side condition on β , which, in our proposed experiment, reads as follows. The single-crystal is oriented such that one of the cubic crystal axes points in the x_3 direction of the specimen, and the other two lie in the $x_1 - x_2$ plane, rotated by 45° with respect

*For comparison, we also consider the diagonal-shear case, where the upper end of the specimen is fixed according to $u(\cdot, L, \cdot) = \gamma(1, 1, 0)$.

to the $x_1 - x_2$ co-ordinate axes. Thus,

$$\begin{aligned} \beta(x) \in \bigg\{ & s(x) \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, s(x) \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ -1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \\ & s(x) \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, s(x) \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ -1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \\ & s(x) \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, s(x) \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \bigg\}, \end{aligned} \quad (2)$$

for almost every $x = (x_1, x_2, x_3) \in \Omega_L$ and some coefficient $s: \Omega_L \rightarrow \mathbb{R}$. Note that there are indeed materials which exhibit such (primary) slip systems (or rotated equivalents[†]), in particular materials with B2 (caesium-chloride) structure, such as the intermetallic compounds Yttrium-Zinc [13] or Nickel-Aluminium.

The article is organized as follows. In the next section we introduce a two-dimensional (sliced) version of our problem, and prove the key energy inequalities. Then, in section 3, we show that the relaxed three-dimensional problem can be reduced to the two-dimensional one, simply by adding up slices. In section 4, we show that a further reduction to a two-dimensional scalar model of plasticity does not, in our set-up with free lateral boundary conditions, yield reasonable energy bounds. Finally, some conclusions and open problems are discussed in section 5.

2 The two-dimensional model

We now introduce a 2-d model which basically corresponds to a vertical slice of the full 3-d model. Once the dimension reduction has been made, we proceed to obtain the desired upper and lower energy bounds.

2.1 Description of the 2-d model

Consider a rectangular specimen which occupies the domain $\overline{\Omega}_L = (0, 1) \times (0, L) \subset \mathbb{R}^2$, and look for a vector displacement $u: \overline{\Omega}_L \rightarrow \mathbb{R}^2$ and a plastic-distortion tensor $\beta: \overline{\Omega}_L \rightarrow \mathbb{R}^{2 \times 2}$ which minimise the linearised-plasticity functional

$$\overline{E}_L(u, \beta) = \int_{\overline{\Omega}_L} |(\nabla u - \beta)_{\text{sym}}|^2 dx + \sigma \int_{\overline{\Omega}_L} |\nabla \times \beta|, \quad (3)$$

subject to the single-slip side condition

$$\beta(x) \propto \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}, \quad (4)$$

for a.e. $x = (x_1, x_2) \in \overline{\Omega}_L$.

The *curl* term appearing in (3) models the energy of GNDs (with σ interpreted as the line energy), and is defined by analogy with the measure-theoretic quantity introduced in [12], such that

[†]There may also exist further Burgers vectors lying within the respective slip planes—we show in section 3 that such considerations are irrelevant to our analysis.

it is continuous with respect to a mollification of β which respects the side condition (4). The most convenient way of explicitly making the definition is in terms of co-ordinates (ξ, η) which are rotated at 45° with respect to the x_i , and hence aligned with the slip directions. Thus, for $\beta \in \text{BV}$, say,

$$\int_{\overline{\Omega}_L} |\nabla \times \beta| = \sup \int_{\overline{\Omega}_L} \phi_{,\xi} \beta_{\xi\eta} + \psi_{,\eta} \beta_{\eta\xi} d\xi d\eta, \quad (5)$$

where the *supremum* is taken over all $\phi, \psi \in C_0^1(\overline{\Omega}_L, [-1, 1])$, and we have used the comma notation for partial derivatives.

Note that, in such rotated co-ordinates, the side condition (4) takes the simpler form

$$\beta(\xi, \eta) \propto \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad (6)$$

for a.e. $(\xi, \eta) \in \overline{\Omega}_L$, which will be extremely useful in the sequel. Also note that, for smooth β , (5) is just the L^1 -norm of the ordinary row-wise curl of β .

Our main goal in what follows will be to obtain lower bounds on \overline{E}_L as the reciprocal aspect ratio, L , is varied, subject to two sets of boundary conditions, corresponding to diagonal and horizontal shear, respectively. The *infimum* of \overline{E}_L will be taken over (u, β) which satisfy the boundary conditions under consideration, and we will write $J_L = \inf \overline{E}_L(\cdot, \cdot)$.

The boundary conditions to be treated are, when expressed in x_i -co-ordinates,

(BC1) $u = \gamma(1, 1)$ at $x_2 = L$ and $u = (0, 0)$ at $x_2 = 0$,

(BC2) $u = \gamma(1, 0)$ at $x_2 = L$ and $u = (0, 0)$ at $x_2 = 0$,

where $\gamma > 0$ is a measure of the fixed average (diagonal or horizontal) shear.

We begin with the following pair of elementary results:

Proposition 2.1. *Under BC1 or BC2, J_L is a monotonically decreasing function of L .*

Proof. Fix $L > 0$, and choose $0 < \delta < L$. Next note that we can write $\overline{\Omega}_{L-\delta} = (\frac{L-\delta}{L}) \overline{\Omega}_L \sqcup A$, where $\text{meas}(A) > 0$. Also note that \overline{E}_L is invariant under an overall scaling of $\overline{\Omega}_L$, via $\hat{u}(\lambda x) = u(x)$, $\hat{\beta}(\lambda x) = \frac{1}{\lambda} \beta(x)$, for a scale-factor λ , say. The result follows by the super-additivity of the energy as a set function. \square

Proposition 2.2. *Under BC1 or BC2, J_L is a left-continuous function of L .*

Proof. Fix $\epsilon, L > 0$, and take a smooth pair (u, β) on $\overline{\Omega}_L$ such that $\overline{E}_L(u, \beta) \leq J_L + \epsilon$. Now scale u and β as in the above proposition to get $(\hat{u}, \hat{\beta})$ defined on $S = (\frac{L-\delta}{L}) \overline{\Omega}_L \subset \overline{\Omega}_{L-\delta}$. Extend $(\hat{u}, \hat{\beta})$ to the whole of $\overline{\Omega}_{L-\delta}$ by constancy in the x_1 -direction, thus preserving the boundary conditions at $x_2 = 0$ and $x_2 = L - \delta$. This construction induces no extra curl on $x_1 = 1 - \frac{\delta}{L}$, and the energy in $\overline{\Omega}_{L-\delta} \setminus S$ tends to zero as $\delta \rightarrow 0$. Hence $\lim_{\delta \rightarrow 0+} J_{L-\delta} \leq J_L + \epsilon$. Since ϵ was arbitrary, we get the desired result. \square

2.2 Diagonal shear

While a diagonal shear would be rather difficult to impose in a real experiment, due to slippage, it turns out that most of the test-function constructions required for horizontal shear have simpler analogues in the **BC1** case which are much easier to explain in the first instance. For this reason, we now present the **BC1** model by way of an introduction to the more complex **BC2** problem.

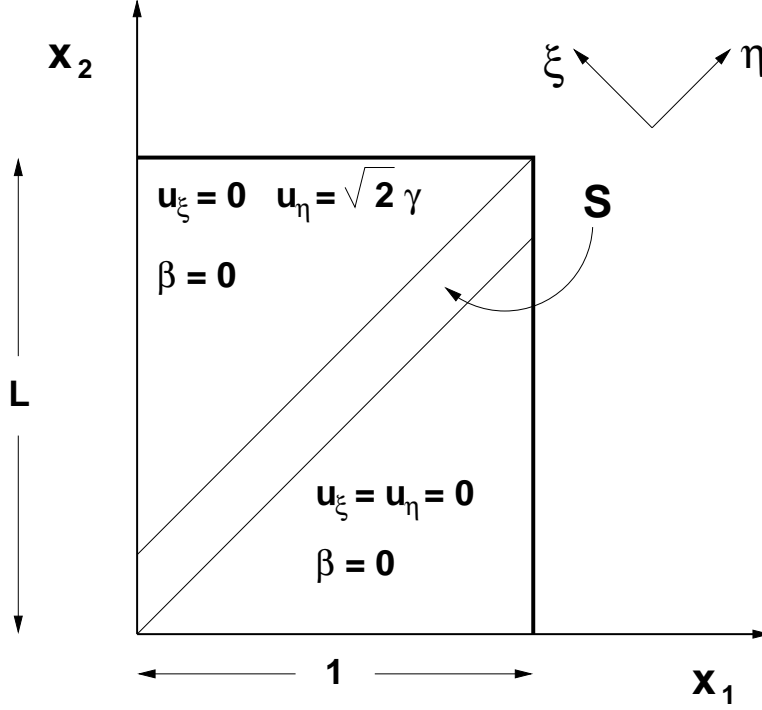


Figure 1: A minimising pair for **BC1** in the case $L > 1$.

In terms of rotated co-ordinates, (ξ, η) , aligned as in Figure 1, the Dirichlet condition of **BC1** at the top boundary becomes $(u_\xi, u_\eta) = \gamma(0, \sqrt{2})$, while, of course, $(u_\xi, u_\eta) = (0, 0)$ at the bottom. Using this, it is easy to construct zero-energy test functions whenever $L > 1$.

Theorem 2.3. *Subject to **BC1**, $L > 1 \Rightarrow J_L = 0$.*

Proof. Take a simple-shear band S , of width ϵ , which just misses the horizontal boundaries, as in Figure 1. Let $u_\xi = u_\eta = \beta = 0$ below S , $u_\xi = 0, u_\eta = \sqrt{2}\gamma, \beta = 0$ above S , and interpolate linearly between the two to ensure that

$$\nabla u = \beta = \begin{pmatrix} 0 & 0 \\ \frac{\sqrt{2}\gamma}{\epsilon} & 0 \end{pmatrix}, \quad (7)$$

on S , in (ξ, η) co-ordinates. Clearly the boundary conditions are satisfied by the resulting test functions, and it is trivial to check that $\overline{E}_L(u, \beta) = 0$. \square

Theorem 2.4. *Subject to **BC1**, $L < 1 \Rightarrow \exists c_L > 0$ such that*

$$\frac{\gamma^2}{L}(1 - L) \leq J_L \leq \min \left\{ \frac{3\gamma^2}{2L}, \frac{\gamma^2}{L}(1 - L) + c_L \sigma \gamma \right\}. \quad (8)$$

Proof. For the lower bound, fix $L < 1$, and choose a pair (u, β) satisfying **BC1**. By (3) and (6), we immediately get

$$\left\| \frac{\partial u_\eta}{\partial \eta} \right\|_{L^2(\overline{\Omega}_L)}^2 + \left\| \frac{\partial u_\xi}{\partial \xi} \right\|_{L^2(\overline{\Omega}_L)}^2 \leq \overline{E}_L(u, \beta). \quad (9)$$

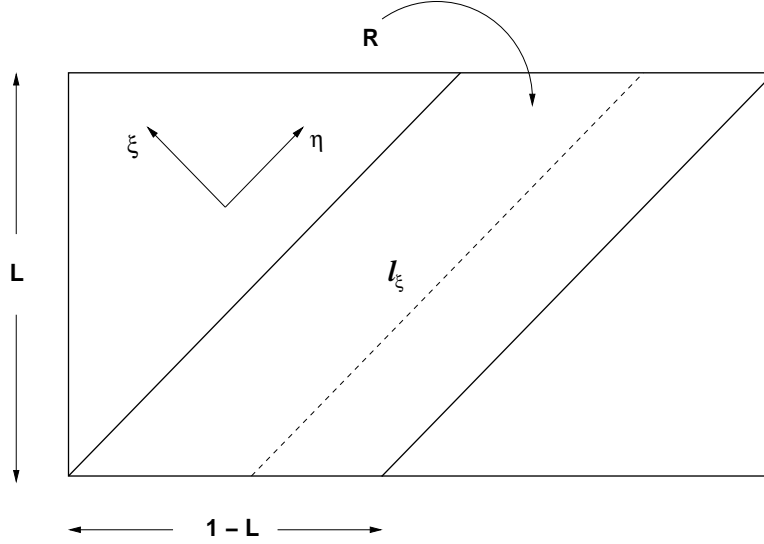


Figure 2: The line l_ξ and the region R used in the lower-bound proof of Theorem 2.4.

Referring to Figure 2, we fix ξ such that the dotted line l_ξ (of constant ξ) lies in the region $R \subset \overline{\Omega}_L$ which is bounded by the two solid diagonals. Now integrate $\frac{\partial u_\eta}{\partial \eta}$ along l_ξ from $u_\eta = 0$ to $u_\eta = \sqrt{2}\gamma$ to get

$$\sqrt{2}\gamma = \int_{l_\xi} \frac{\partial u_\eta}{\partial \eta} d\eta, \quad (10)$$

and integrate over all such $l_\xi \subset R$, to arrive at

$$\gamma(1-L) = \iint_R \frac{\partial u_\eta}{\partial \eta} d\eta d\xi. \quad (11)$$

Using $|R| = L(1-L)$, along with the usual $L^2 \hookrightarrow L^1$ embedding, we get

$$\gamma(1-L) \leq \left\| \frac{\partial u_\eta}{\partial \eta} \right\|_{L^1(R)} \leq (L(1-L))^{\frac{1}{2}} \left\| \frac{\partial u_\eta}{\partial \eta} \right\|_{L^2(R)}. \quad (12)$$

Hence, by (9), $\overline{E}_L(u, \beta) \geq \gamma^2(1-L)/L$, as required.

For the upper bound, first note that the first member of the upper-bound set is attained by the minimising (linear) purely elastic deformation. Next, we get arbitrarily close to the second member with the following construction, which is depicted in Figure 3.

Divide $\overline{\Omega}_L$ into five regions: R_ϵ (a slightly narrower version of R from Figure 2), two transition layers of width ϵ centred on the corner-diagonals of constant ξ , and two triangles which surround the R_ϵ /transition-layer sandwich.

Set $u_\xi = 0$ on $\overline{\Omega}_L$, and, on R_ϵ , determine u_η , for each fixed ξ , by linearly interpolating between the Dirichlet conditions at $x_2 = 0$ and $x_2 = L$, and set $\beta_{\eta\xi} = \frac{\partial u_\eta}{\partial \xi}$. On the upper and lower triangles take $\beta = 0$ and, respectively, $u_\eta = \sqrt{2}\gamma$ and $u_\eta = 0$. This gives a total elastic energy away from the transition layers amounting to $\frac{\gamma^2}{L}(1-L-\sqrt{2}\epsilon)$, and zero plastic energy.

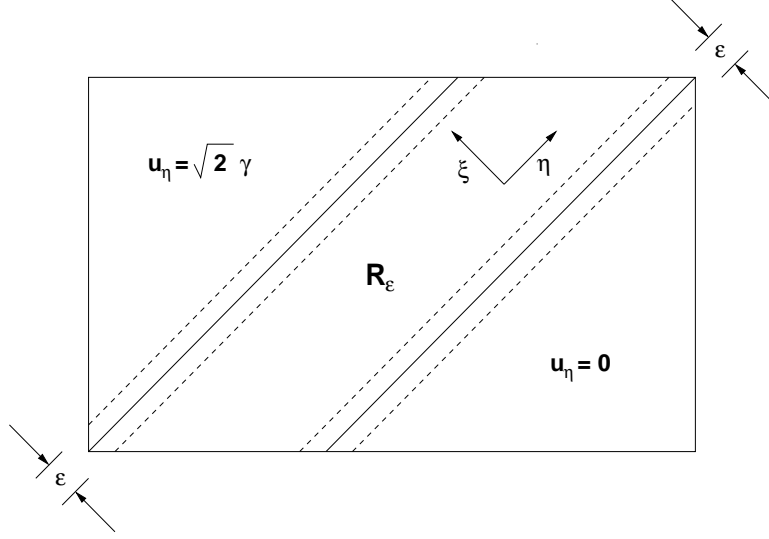


Figure 3: Construction used in the upper-bound proof of Theorem 2.4.

On the transition layers, (u, β) can be chosen such that the elastic energy is small, and the plastic energy is $\mathcal{O}(\sigma\gamma)$. To be specific, divide the upper transition layer into a small triangle, A , in the bottom left corner of $\overline{\Omega}_L$, and a narrow strip, B (see Figure 4a). Then, by analogy with the proof of Theorem 2.5 (see below), we can make the energy in A arbitrarily small, as follows. Thus, take a function $u_\eta^\beta(\xi)$ with (piecewise) ξ^α -shape, representing a steep transition from 0 to $\frac{\gamma}{\sqrt{2}}$ along the diagonal boundary of A . Then set $\beta = \nabla u_\eta^\beta$, put $v = u_\eta - u_\eta^\beta$ and minimise $\|\nabla v\|_{L^2(A)}$, subject to $u_\eta = 0$ on $x_2 = 0$ and $u_\eta = u_\eta^\beta$ on the diagonal boundary of A . This can be done by reflecting A about its vertical boundary and solving the Laplace equation for v on the resulting domain, which gives arbitrarily small energy as $\alpha \rightarrow 0$.

Meanwhile, on B , interpolate u_η between the u_η^β -profile at the boundary with A and the Dirichlet condition at $x_2 = L$, for each fixed ξ , and accommodate the resulting twist by setting $\beta_{\eta\xi} = \frac{\partial u_\eta}{\partial \xi}$.

The result of this is that we have, for small enough $\alpha(\epsilon)$, $\mathcal{O}(\epsilon)$ elastic energy and $\mathcal{O}(\sigma\gamma)$ plastic energy on the upper transition layer. Clearly, an analogous construction works on the lower transition layer, and hence, letting $\epsilon \rightarrow 0$, the desired upper bound follows. \square

An interesting question is whether J_L jumps from zero to a strictly positive number as L decreases through unity: we now answer this question in the negative.

Theorem 2.5. *Subject to BC1, $J_1 = 0$, and hence, by Proposition 2.2, J_L is continuous at $L = 1$.*

To prove Theorem 2.5, we need the aid of the following Lemma.

Lemma 2.6. *The family of functions $f_\alpha(x) = 1 - x^\alpha$, $\alpha \in [0, 1]$, lies in $H^{\frac{1}{2}}(0, 1)$, and $\|f_\alpha\|_{H^{\frac{1}{2}}(0, 1)} \searrow 0$ as $\alpha \rightarrow 0^+$. In particular, $H^{\frac{1}{2}}(0, 1)$ is not embedded in $L^\infty(0, 1)$, since $\|f_\alpha\|_{L^\infty(0, 1)} = 1$ for $\alpha \in [0, 1]$. Moreover, the reflected functions $\tilde{f}_\alpha(x) = 1 - (\text{sgn}(x)x)^\alpha$ lie in $H^{\frac{1}{2}}(-1, 1)$, and also $\|\tilde{f}_\alpha\|_{H^{\frac{1}{2}}(-1, 1)} \searrow 0$ as $\alpha \rightarrow 0^+$.*

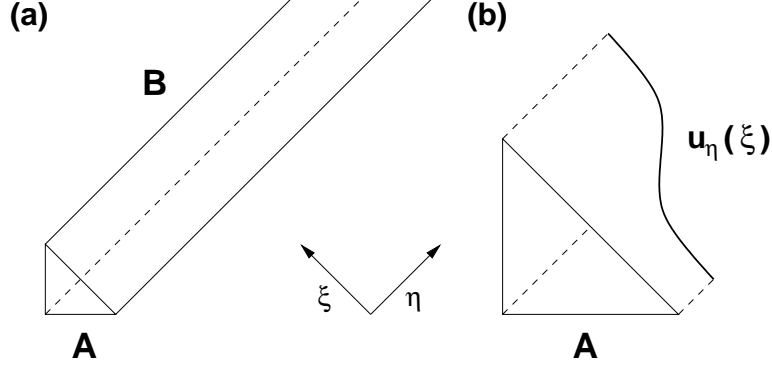


Figure 4: Construction used in the upper-bound proof of Theorem 2.4. **(a)** The upper transition layer, comprising regions A and B , **(b)** Profile of u_η on the diagonal boundary of A .

Proof. Clearly, $f_\alpha \in L^2$, $\|f_\alpha\|_{L^2} \searrow 0$ and $\|f_\alpha\|_{L^\infty} = 1$. Now, turning to the $H^{\frac{1}{2}}$ semi-norm, we define

$$Q(\alpha) = |f_\alpha|_{H^{\frac{1}{2}}}^2 = \int_0^1 \int_0^1 \frac{(x^\alpha - y^\alpha)^2}{(x - y)^2} dx dy, \quad P(\alpha, x, y) = (x^\alpha - y^\alpha)^2, \quad (13)$$

for $(\alpha, x, y) \in (0, 1)^3$.

Thus, $Q(0) = 0$, $Q(1) = 1$, and $P(0) = 0$. Moreover,

$$\frac{\partial P}{\partial \alpha} = 2(x^\alpha - y^\alpha)(x^\alpha \ln x - y^\alpha \ln y) \geq 0, \quad (14)$$

so that $P(\cdot, x, y)$ is increasing, and clearly $P(\alpha, x, y) \rightarrow P(0, x, y) = 0$ as $\alpha \rightarrow 0+$. Thus, by dominated convergence, $Q(\alpha) \rightarrow 0$ as $\alpha \rightarrow 0+$, as required.

For \bar{f}_α , the semi-norm integral can be split into two ‘diagonal’ terms, which can be handled as above, and two ‘cross’ terms, given by

$$\int_{-1}^0 \int_0^1 \frac{(x^\alpha - (\text{sgn}(y)y)^\alpha)^2}{(x - y)^2} dx dy = \int_0^1 \int_0^1 \frac{(x^\alpha - z^\alpha)^2}{(x + z)^2} dx dz, \quad (15)$$

where we changed variables via $z = -y$ in the final equality. Clearly, the last integral is smaller than $Q(\alpha)$, and increasing w.r.t. α , which gives the required result. \square

Proof of Theorem 2.5. Here it will be convenient to align the rotated (ξ, η) co-ordinates as in Figure 5, with the origin taken to be at the centre of $\bar{\Omega}_1$.

Given this, consider the sigmoid function $g_\alpha(\xi)$ defined by

$$g_\alpha(\xi) = \frac{\gamma}{\sqrt{2}} \left(1 - \text{sgn}(\xi) \left(\text{sgn}(\xi) \sqrt{2} \xi \right)^\alpha \right) \quad (16)$$

on the interval $(-1/\sqrt{2}, 1/\sqrt{2})$, which represents a steep transition from 0 to $\sqrt{2}\gamma$ (see Figure 6).

Now define, in the (ξ, η) -frame, $u^\beta = (0, g_\alpha(\xi))$, and put

$$\beta = \nabla u^\beta = \begin{pmatrix} 0 & 0 \\ g'_\alpha(\xi) & 0 \end{pmatrix} \quad (17)$$

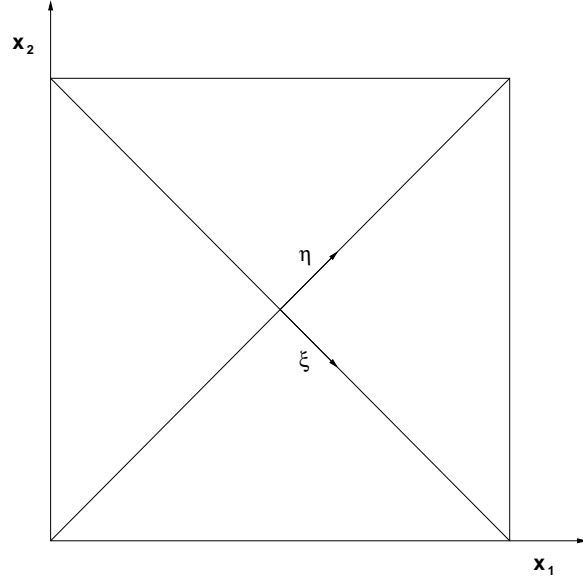


Figure 5: Orientation of the (ξ, η) co-ordinates on $\overline{\Omega}_1$ used in the proof of Theorem 2.5.

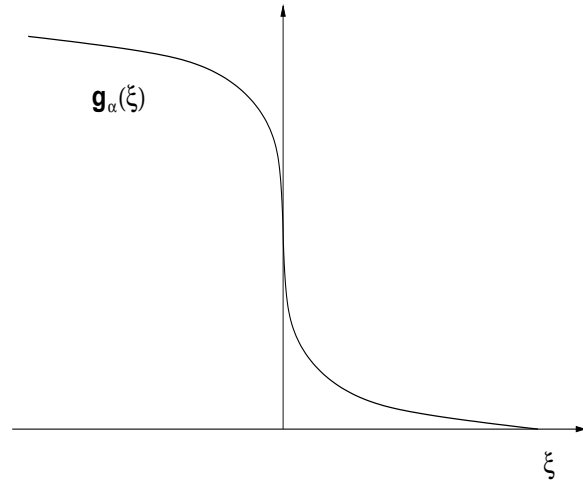


Figure 6: The function $g_\alpha(\xi)$ used in the proof of Theorem 2.5.

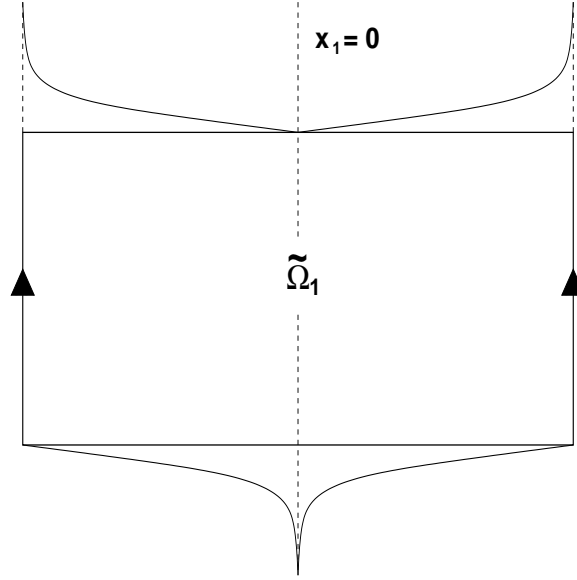


Figure 7: Shape of the Dirichlet data on $\tilde{\Omega}_1$ used in the proof of Theorem 2.5.

Thus, β is curl-free, and, for a general test function u , we define $v = u - u^\beta$ and set $v_\xi = 0$ ($\Leftrightarrow u_\xi = 0$, consistent with **BC1**). The aim is now to show that the minimum of $\|\nabla v_\eta\|_{L^2}$, subject to the boundary conditions

$$v_\eta(\xi, \eta) = \begin{cases} -g_\alpha(\xi) & : x_2 = 0 \\ \sqrt{2}\gamma - g_\alpha(\xi) & : x_2 = 1 \end{cases}, \quad (18)$$

tends to zero as $\alpha \rightarrow 0$: this will be achieved by using the continuity of the (Dirichlet) solution operator to Laplace's equation, $\Delta v_\eta = 0$.

In order to do this, it is convenient to consider reflected (about $x_1 = 0$) Dirichlet data on the double of $\tilde{\Omega}_1$, with resulting lateral boundaries then identified to make a cylinder. Thus, we work on the manifold $\tilde{\Omega}_1 = \mathbb{S}^1 \times (0, 1)$, with boundary $\mathbb{S}^1 \sqcup \mathbb{S}^1$, and the Dirichlet data for v_η on each boundary \mathbb{S}^1 have the same shape as \bar{f}_α from Lemma 2.6 (see Figure 7). By the symmetry of this data, and invariance of $\Delta v_\eta = 0$ under reflections, we see that solving the Dirichlet problem on $\tilde{\Omega}_1$, for a function still denoted by v_η , gives a solution of the mixed Dirichlet/Neumann problem on $\bar{\Omega}_1$. Now, Proposition 1.7 on p.307 of [14] tells us that the solution map to the Dirichlet problem on $\tilde{\Omega}_1$ takes $H^{\frac{1}{2}}(\partial\tilde{\Omega}_1)$ continuously into $H^1(\tilde{\Omega}_1)$, while our Lemma 2.6 gives, modulo trivial scalings applied to \bar{f}_α , $\|\text{Tr}(v_\eta)\|_{H^{\frac{1}{2}}(\partial\tilde{\Omega}_1)} \rightarrow 0$ as $\alpha \rightarrow 0$, as desired. \square

Remark 2.7. In the above construction, if we use a piecewise-linear transition function with 3-pieces, rather than g_α , then we get an $\mathcal{O}(\gamma^2)$ amount of energy, as can easily be checked, using the trace inequality.

2.3 Horizontal shear

In this section we minimise \bar{E}_L subject to the horizontal-shear condition **BC2**. In a (ξ, η) -frame aligned as in Figure 1, the Dirichlet condition at $x_2 = L$ is $(u_\xi, u_\eta) = \gamma(-1/\sqrt{2}, 1/\sqrt{2})$, while

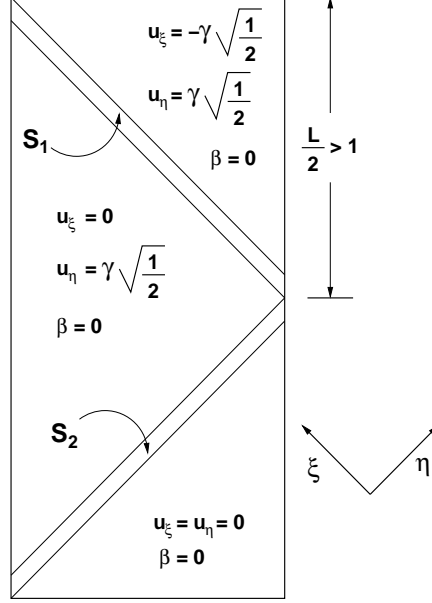


Figure 8: Zero-energy construction for Theorem 2.8.

$(u_\xi, u_\eta) = (0, 0)$ at $x_2 = 0$.

Theorem 2.8. *Subject to **BC2**, $L > 2 \Rightarrow J_L = 0$.*

Proof. We use basically the same construction as in the proof of Theorem 2.3, except that here, since $L > 2$, there is enough room to fit two alternating, non-intersecting shear bands into $\overline{\Omega}_L$, each of which misses the Dirichlet boundary (see Figure 8).

To be explicit, we take two shear bands, given by $S_1 = \{x_1 + x_2 \leq L\} \cap \{x_1 + x_2 \geq 1 + L/2\}$ and $S_2 = \{x_2 - x_1 \geq 0\} \cap \{x_2 - x_1 \leq -1 + L/2\}$, which just touch at the lateral boundary $x_1 = 1$. Above S_1 set $u_\xi = -\gamma/\sqrt{2}$, $u_\eta = \gamma/\sqrt{2}$, $\beta = 0$, between S_1 and S_2 set $u_\xi = 0$, $u_\eta = \gamma/\sqrt{2}$, $\beta = 0$, and below S_2 put $u_\xi = u_\eta = \beta = 0$. Then linearly interpolating u across S_1 and S_2 , and requiring that $\nabla u = \beta$ on $S_1 \cup S_2$ clearly gives a pair of test functions which satisfy **BC2**, and for which $\overline{E}_L = 0$. \square

A certain amount of energy is required to produce a horizontal shear when L is sufficiently small, which is the content of the following two theorems.

Theorem 2.9. *Subject to **BC2**, $L < 1 \Rightarrow \exists c_L > 0$ such that*

$$\frac{\gamma^2}{2L}(1-L) \leq J_L \leq \min \left\{ \frac{\gamma^2}{2L}, \frac{\gamma^2}{2L}(1-L) + c_L \sigma \gamma \right\} \quad (19)$$

Proof. The proof is very similar to that of Theorem 2.4.

Thus, for the lower bound, take a test pair (u, β) , and integrate $\frac{\partial u_\eta}{\partial \eta}$ over the strip R (see Figure 2), to get

$$\left\| \frac{\partial u_\eta}{\partial \eta} \right\|_{L^2}^2 \geq \frac{\gamma^2(1-L)}{4L}, \quad (20)$$

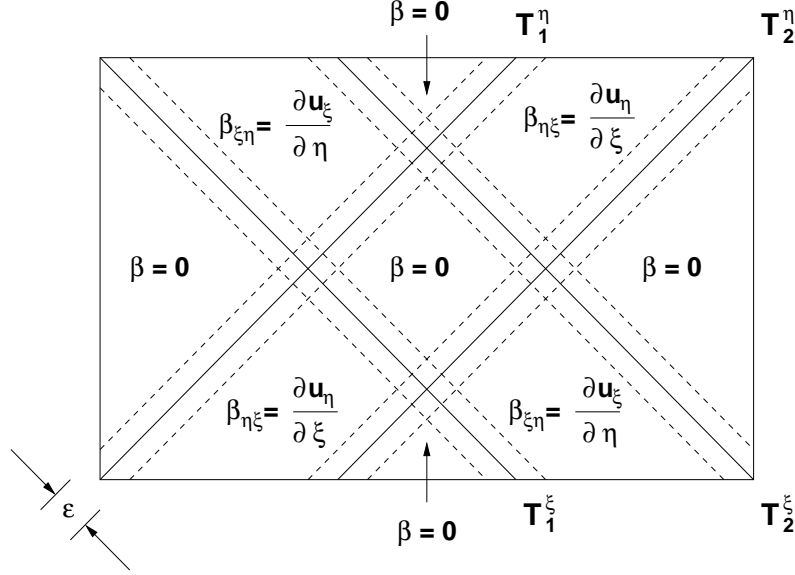


Figure 9: Transition layers used in the proof of Thm 2.9.

and integrate $\frac{\partial u_\xi}{\partial \xi}$ over an analogous strip pointing in the ξ -direction to get the same estimate for $\left\| \frac{\partial u_\xi}{\partial \xi} \right\|_{L^2}$. Hence, $\overline{E}_L(u, \beta) \geq \gamma^2(1 - L)/2L$, as required.

For the upper bound, it is easy to see that the first member of the upper-bound set in (19) is attained by the minimising purely elastic deformation, while the second member can be approached by a construction similar to, but more complicated than, that used in the proof of Thm 2.4, the difference being that here we need two transition layers for each of u_ξ and u_η , and we have to take a little care on the regions where they intersect.

Thus, referring to Figure 9, we define, for $i = 1, 2$, the transition layers T_i^η to be narrow strips of width ϵ , centred on the corner-diagonals of constant ξ , and T_i^ξ to be strips of the same width, but centred on the corner-diagonals of constant η . Between the T_i^η , u_η is obtained by linear interpolation between the Dirichlet conditions, in the η direction, while above and below the T_i^η -sandwich, u_η is set equal to the appropriate Dirichlet condition. The other component of the displacement, u_ξ , is obtained on the complement of the T_i^ξ in an analogous manner.

Next, u_η is defined on T_1^η as follows. Divide the part of T_1^η below the intersection with T_1^ξ into two parts, A and B' , such that A is the same as in Figure 3 and B' is a truncated version of B (see Figure 10). Define u_η on A in exactly the same way as in Thm 2.4 with $\alpha > 0$ small and fixed, and, for each fixed ξ , interpolate from the diagonal boundary of A up to the unique linear profile on the upper constant- η boundary of B' which connects u_η continuously across T_1^η . On the remainder of T_1^η , define u_η by interpolating up to the Dirichlet condition at $x_2 = L$, for each fixed ξ .

On T_2^η , u_η is determined by a trivial symmetry transformation applied to u_η on T_1^η , and likewise for u_ξ on the T_i^ξ . For the plastic distortion, let $\beta = \nabla u^\beta$ on A , set $\beta = 0$ on $T_1^\eta \cap T_i^\xi$, and on the rest of T_1^η let $\beta_{\eta\xi} = \frac{\partial u_\eta}{\partial \xi}$. Define β on the remaining transition layers by symmetry, and otherwise by appealing to Figure 9.

As a result of this, there is very little elastic energy on the transition layers, while the plastic energy is concentrated there (particularly on the boundaries). More precisely, we have $\left\| \frac{\partial u_\eta}{\partial \eta} \right\|_{L^2}^2 =$

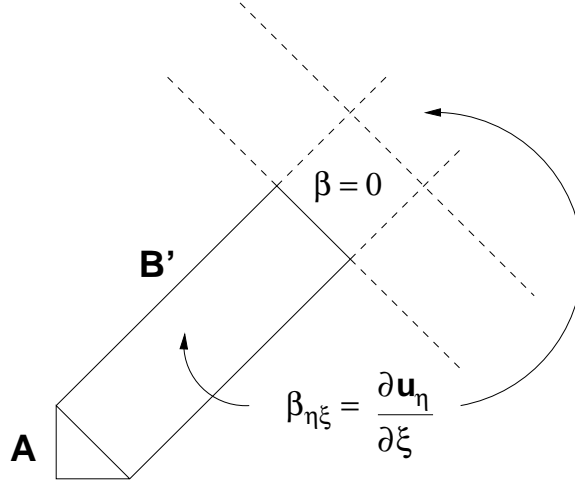


Figure 10: Subsets of T_1^η used in the proof of Thm 2.9.

$\mathcal{O}(\epsilon)$ on T_i^η and $\|\frac{\partial u_\xi}{\partial \xi}\|_{L^2}^2 = \mathcal{O}(\epsilon)$ on T_i^ξ , provided $\alpha(\epsilon)$ was chosen small enough, while, by the symmetry of the construction, $\frac{\partial u_\eta}{\partial \xi} + \frac{\partial u_\xi}{\partial \eta} = \mathcal{O}(1)$, pointwise, on the transition-layer intersections. Also note that, by symmetry, $\frac{\partial u_\eta}{\partial \xi} + \frac{\partial u_\xi}{\partial \eta} = 0$ on the central square, where $\beta = 0$, and thus there is no off-diagonal elastic energy there.

Finally, it is easy to see that all the contributions to the plastic energy are $\mathcal{O}(\sigma\gamma)$, and hence, for our test functions,

$$\overline{E}_L(u, \beta) = \frac{\gamma^2}{2L}(1 - L) + \mathcal{O}(\sigma\gamma) + \mathcal{O}(\epsilon), \quad (21)$$

so that, letting $\epsilon \rightarrow 0$, the desired upper bound follows. \square

We have to work a little harder to prove strict positivity of the energy in the intermediate case $1 < L < 2$.

Theorem 2.10. *Subject to **BC2**, $1 < L < 2 \Rightarrow \exists c_L > 0$ such that*

$$\frac{c_L \sigma \gamma^2}{\sigma + \sqrt{\sigma^2 + 2c_L \gamma^2}} \leq J_L \leq \min \left\{ \frac{\gamma^2}{2L}, 2\sqrt{2}\gamma\sigma \right\}. \quad (22)$$

Proof. For the lower bound, we combine a recent generalisation of Korn's inequality from [15] which is nicely adapted to our energy functional with a Lemma from [12] which allows us to control (one component of) β via the curl, provided the single-slip condition is satisfied.

First, let $1 < L < 2$, and, for test functions (u, β) satisfying **BC2**, we define the average-symmetric tensor A via

$$A(u, \beta) = (\nabla u - \beta) - \frac{1}{|\overline{\Omega}_L|} \int_{\overline{\Omega}_L} (\nabla u - \beta)_{\text{skew}} dx. \quad (23)$$

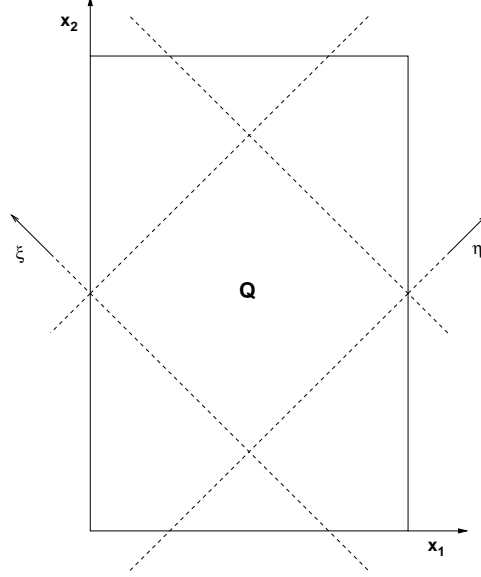


Figure 11: The region Q used in the proof of Theorem 2.10.

Then, by Theorem 11 of [15], there exists a constant $C(\overline{\Omega}_L)$ such that [‡]

$$\int_{\overline{\Omega}_L} |A_{\text{skew}}|^2 dx \leq C \left(\int_{\overline{\Omega}_L} |A_{\text{sym}}|^2 dx + \|\nabla \times A\|_{L^1(\overline{\Omega}_L)}^2 \right), \quad (24)$$

and hence there exists a constant, skew-symmetric matrix $K(u, \beta)$ such that

$$\int_{\overline{\Omega}_L} |(\nabla u - \beta) - K(u, \beta)|^2 \leq C \overline{E}_L(u, \beta) \left(1 + \frac{\overline{E}_L(u, \beta)}{\sigma^2} \right). \quad (25)$$

Now, consider the square $Q \subset \overline{\Omega}_L$, of side $\frac{1}{\sqrt{2}}$, which is bounded by the lines $\{x_1 + x_2 = L/2\}$, $\{x_2 - x_1 = -1 + L/2\}$, $\{x_1 + x_2 = 1 + L/2\}$ and $\{x_2 - x_1 = L/2\}$ (See Figure 11): for convenience, we have put the origin of the (ξ, η) -co-ordinates at the bottom corner of Q .

By analogy with the proof of Lemma 4.3 of [12], we define the following subsets of Q :

$$\omega^{(\xi)} = \{ \xi \in (0, 1) : \beta_{\eta\xi}(\xi, \eta) \neq 0 \text{ for a.e. } \eta \in (0, 1) \}, \quad (26)$$

$$\omega^{(\eta)} = \{ \eta \in (0, 1) : \beta_{\xi\eta}(\xi, \eta) \neq 0 \text{ for a.e. } \xi \in (0, 1) \}, \quad (27)$$

and, from the side condition (4), we conclude that at least one of $\omega^{(\xi)}$ and $\omega^{(\eta)}$ must be a null set. For the remainder of the proof, we may assume w.l.o.g. that $\omega^{(\eta)}$ is a null set.

Let

$$P = \overline{\Omega}_L \cap \left\{ \frac{L}{2} \leq x_1 + x_2 \leq 1 + \frac{L}{2} \right\}, \quad (28)$$

so that P is, so to speak, the extension of Q in the ξ -direction.

[‡]Note that, at the time of writing, (24) is only known to hold in 2-d, although analogous inequalities in higher dimensions have been conjectured by Neff *et al.*[16].

Then, since $\omega^{(\eta)}$ is null, we obtain

$$\|\beta_{\xi\eta}\|_{L^1(P)} \leq C \|\partial_\xi \beta_{\xi\eta}\|_{L^1(P)} \leq \frac{C}{\sigma} \overline{E}_L(u, \beta), \quad (29)$$

and it follows from (6), (25), (29) and $L^2 \hookrightarrow L^1$ embedding that,

$$\left\| \frac{\partial u_\xi}{\partial \xi} \right\|_{L^1(P)}^2 \leq C \overline{E}_L \quad (30)$$

and

$$\left\| \frac{\partial u_\xi}{\partial \eta} - K_{\xi\eta} \right\|_{L^1(P)}^2 \leq C \overline{E}_L \left(1 + \frac{\overline{E}_L}{\sigma^2} \right) + \|\beta_{\xi\eta}\|_{L^1(P)}^2 \quad (31)$$

$$\leq C \overline{E}_L \left(1 + \frac{\overline{E}_L}{\sigma^2} \right). \quad (32)$$

Define strips $T_1, T_2 \subset P$ by

$$T_1 = P \cap \{x_1 + x_2 \leq 1\}, \quad T_2 = P \cap \{x_1 + x_2 \geq L\}, \quad (33)$$

such that T_1 intersects the bottom boundary, and T_2 the top boundary, in a set of length $1 - L/2$.

The strategy now is to show that

$$\|u_\xi\|_{L^1(T_1)} \leq C \overline{E}_L^{\frac{1}{2}}, \quad (34)$$

$$\|u_\xi + \gamma/\sqrt{2}\|_{L^1(T_2)} \leq C \overline{E}_L^{\frac{1}{2}}, \quad (35)$$

$$K_{\xi\eta}(u, \beta) = \mathcal{O}(\overline{E}_L^{\frac{1}{2}}). \quad (36)$$

Then, integrating $\frac{\partial u_\xi}{\partial \eta}$ between T_1 and T_2 will give a lower bound on $K_{\xi\eta}$, and a contradiction if \overline{E}_L is too small relative to the average shear γ .

We begin by integrating $\frac{\partial u_\xi}{\partial \xi}$ from $(\xi_0(\eta), \eta)$ on the $x_2 = 0$ boundary of T_1 to the point (ξ, η) in the interior (see Figure 12), to get

$$u_\xi(\xi, \eta) = \int_{\xi_0}^{\xi} \frac{\partial u_\xi}{\partial \xi}(\xi', \eta) d\xi', \quad (37)$$

which, upon integration over $(\xi, \eta) \in T_1$, gives

$$\iint_{T_1} |u_\xi| d\xi d\eta \leq \iint_{T_1} \int_{\xi_0(\eta)}^{\xi} \left| \frac{\partial u_\xi}{\partial \xi} \right|(\xi', \eta) d\xi' d\xi d\eta \quad (38)$$

$$\leq C \left\| \frac{\partial u_\xi}{\partial \xi} \right\|_{L^1(\overline{\Omega}_L)} \quad (39)$$

$$\leq C \overline{E}_L^{\frac{1}{2}}, \quad (40)$$

and therefore (34) holds. The estimate (35) follows by an analogous integration on T_2 .

For the upper bound on $K_{\xi\eta}$, consider the small triangle $R_1 = T_1 \cap \{x_1 - x_2 \geq \frac{L}{2}\}$ next to the $x_2 = 0$ boundary (Figure 13b).

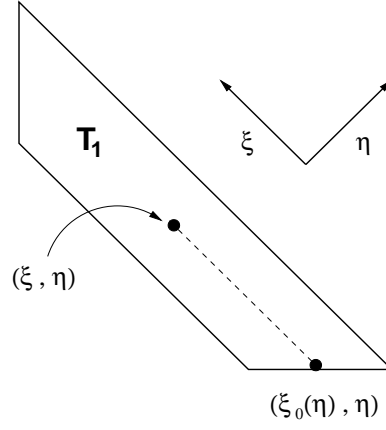


Figure 12: Construction used in the proof of Eq.(34).

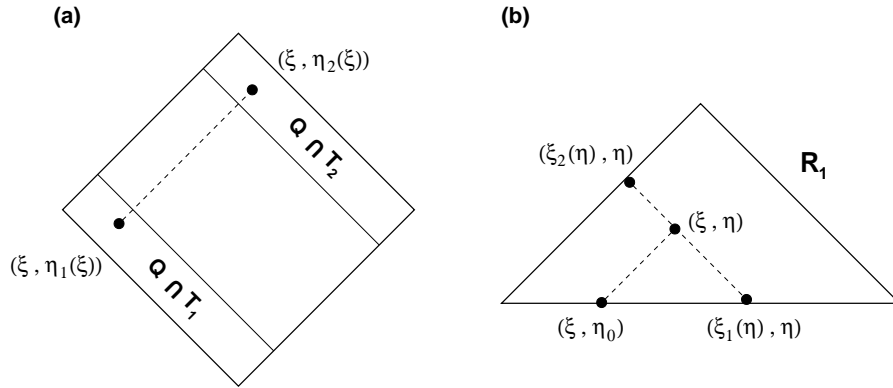


Figure 13: Constructions for the lower (a) and upper (b) bounds on $K_{\xi\eta}$ in Thm 2.10.

Integrate $\frac{\partial u_\xi}{\partial \eta}$ from $x_2 = 0$ to the point (ξ, η) , holding ξ fixed:

$$u_\xi(\xi, \eta) = \int_{\eta_0}^{\eta} \frac{\partial u_\xi}{\partial \eta}(\xi, \eta') d\eta', \quad (41)$$

then integrate (41) between $\xi_1(\eta)$ and $\xi_2(\eta)$, and sum over all line segments (ξ_1, ξ_2) lying in R_1 , to get

$$\iint_{R_1} u_\xi(\xi, \eta) d\xi d\eta = \int_{\eta_1}^{\eta_2} \int_{\xi_1(\eta)}^{\xi_2(\eta)} \int_{\eta_0(\xi)}^{\eta} \frac{\partial u_\xi}{\partial \eta}(\xi, \eta') d\eta' d\xi d\eta, \quad (42)$$

where $[\eta_1, \eta_2] = \Pi_\eta(R_1)$, and Π_η denotes projection onto the η -axis.

Adding and subtracting $K_{\xi\eta}$ to the integrand on the rhs of (42), and using (32) and (34), we arrive at

$$|K_{\xi\eta}| \leq C \overline{E}_L^{\frac{1}{2}} \left(1 + \left(1 + \frac{2\overline{E}_L}{\sigma^2} \right)^{\frac{1}{2}} \right). \quad (43)$$

For the lower bound on $K_{\xi\eta}$, we work on the square Q , and, in particular, the subsets $Q \cap T_i$ thereof (see Figure 13b).

Firstly, we integrate $\frac{\partial u_\xi}{\partial \eta}$ between the two points $(\xi, \eta_1(\xi)) \in Q \cap T_1$ and $(\xi, \eta_2(\xi)) \in Q \cap T_2$:

$$\int_{\eta_1(\xi)}^{\eta_2(\xi)} \frac{\partial u_\xi}{\partial \eta}(\xi, \eta') d\eta' = u_\xi(\xi, \eta_2) - u_\xi(\xi, \eta_1). \quad (44)$$

Then, we integrate (44) over $\xi \in \Pi_\xi(Q)$, $\eta_1 \in \Pi_\eta(T_1)$ and $\eta_2 \in \Pi_\eta(T_2)$, to arrive at

$$\iiint \frac{\partial u_\xi}{\partial \eta}(\xi, \eta') d\eta' d\xi d\eta_1 d\eta_2 = \frac{1}{\sqrt{2}} \left(1 - \frac{L}{2} \right) \left(\iint_{T_2} u_\xi d\xi d\eta_2 - \iint_{T_1} u_\xi d\xi d\eta_1 \right). \quad (45)$$

Thus, adding and subtracting $K_{\xi\eta}$ from the integrand on the lhs of (45), and using (32), (34) and (35), gives us

$$|K_{\xi\eta}| \geq C \left(\frac{\gamma}{\sqrt{2}} - \overline{E}_L^{\frac{1}{2}} \left(1 + \left(1 + \frac{2\overline{E}_L}{\sigma^2} \right)^{\frac{1}{2}} \right) \right), \quad (46)$$

which, together with (43), implies

$$\overline{E}_L^{\frac{1}{2}} \left(1 + \left(1 + \frac{2\overline{E}_L}{\sigma^2} \right)^{\frac{1}{2}} \right) \geq C\gamma. \quad (47)$$

Squaring, and using $(a+b)^2 \leq 2(a^2 + b^2)$ plus the quadratic formula, leads to the required lower bound on J_L .

For the upper bound on J_L , we note that the first member of the upper-bound set in (2.10) is attained by the minimising purely elastic deformation satisfying **BC2**, while the second member is attained by a simple crossing-shear-band construction, as follows.

Referring to Figure 14, inscribe, in $\overline{\Omega}_L$, crossing shear bands S_1 and S_2 which just miss the Dirichlet boundaries, and which have width $\frac{1}{\sqrt{2}}(L-1)$. Then define u_ξ and u_η by linearly interpolating between the boundary conditions across the respective S_i . Finally, set $\beta = \nabla u$ on $\overline{\Omega}_L \setminus (S_1 \cap S_2)$ and $\beta = 0$ on $S_1 \cap S_2$. An easy calculation shows that the elastic energy vanishes, while the plastic energy is given by $2\sqrt{2}\gamma\sigma$, as required. \square

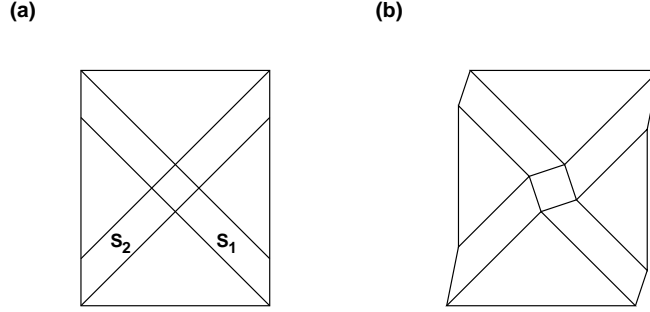


Figure 14: Upper-bound construction for Thm 2.10 (a) in the reference configuration, and (b) the deformed configuration.

Remark 2.11. If the single-slip condition is dropped then $J_L = 0$ for $L > 1$, by essentially the same construction as in Figure 14, the difference being that we may take $\beta = \nabla u$ on the whole of $\bar{\Omega}_L$, and not just away from the shear-band intersection.

Finally, we show that, as in the diagonal-shear case, the transition from zero to positive energy is continuous.

Theorem 2.12. *Subject to BC2, $L = 2 \Rightarrow J_L = 0$.*

Proof. The proof is similar to that of Theorem 2.5.

Take $L = 2$, and let the (ξ, η) -co-ordinates be centred at the mid-point of the right-hand lateral boundary, as shown in Figure 15.

We construct test functions (u^β, β) as follows. On $\{\xi > 0, \eta < 0\}$ let $(u_\xi^\beta, u_\eta^\beta) = \gamma(0, 1/\sqrt{2})$ and $\beta = 0$, on $\{\xi > 0, \eta > 0\}$ let

$$u_\xi^\beta = -\frac{\gamma}{\sqrt{2}} \left(\sqrt{2}\eta \right)^\alpha, \quad u_\eta^\beta = \frac{\gamma}{\sqrt{2}}, \quad \beta = \nabla u^\beta, \quad (48)$$

and on $\{\xi < 0, \eta < 0\}$ let

$$u_\xi^\beta = 0, \quad u_\eta^\beta = \frac{\gamma}{\sqrt{2}} \left(1 - (-\sqrt{2}\xi)^\alpha \right), \quad \beta = \nabla u^\beta, \quad (49)$$

for $\alpha \in [0, 1]$.

Clearly, $\nabla \times \beta = 0$, and, writing $v = u - u^\beta$ as usual, we wish to make $\bar{E}_L = \|(\nabla v)_{\text{sym}}\|_{L^2}^2$ arbitrarily small by letting $\alpha \rightarrow 0$, subject to the boundary conditions

$$(v_\xi, v_\eta) = \begin{cases} \left(\frac{\gamma}{\sqrt{2}} ((\sqrt{2}\eta)^\alpha - 1), 0 \right) & : x_2 = 2, \\ \left(0, \frac{\gamma}{\sqrt{2}} (-1 + (-\sqrt{2}\xi)^\alpha) \right) & : x_2 = 0 \end{cases}. \quad (50)$$

Since we have

$$\|(\nabla v)_{\text{sym}}\|_{L^2}^2 \leq C (\|\nabla v_\xi\|_{L^2}^2 + \|\nabla v_\eta\|_{L^2}^2), \quad (51)$$

it is enough to show that $\|\text{Tr}(v)\|_{H^{\frac{1}{2}}(\partial\bar{\Omega}_2)} \rightarrow 0$ as $\alpha \rightarrow 0$. The proof of this follows just as in the diagonal-shear case. \square

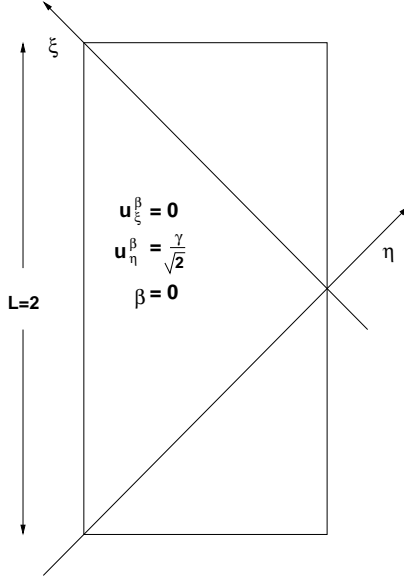


Figure 15: Orientation of (ξ, η) -co-ordinates used in the proof of Theorem 2.12.

3 Extension to 3-d: B2 crystals

A sceptical reader might be tempted to dismiss our 2-d model as somewhat artificial, but in fact the results of section 2 carry over almost immediately to the case of crystals with *B2* symmetry.

As described in the introduction, two of the slip-plane normals in the B2 crystal are aligned with the (ξ, η) -axes, as before, and the third is aligned with the ζ (resp. x_3)-axis, which is taken to be pointing out of the page.

In co-ordinates x_i aligned with the shear-sample faces, the domain occupied by the crystal is taken to be $\Omega_L = (0, 1) \times (0, L) \times (0, 1)$, and we impose a horizontal shear of magnitude γ , such that the boundary conditions take the form

$$u = \gamma(1, 0, 0) \quad \text{at} \quad x_2 = L, \quad u = (0, 0, 0) \quad \text{at} \quad x_2 = 0. \quad (52)$$

For the purposes of deriving the required lower energy bound, the single-slip side condition on the plastic distortion $\beta: \Omega_L \rightarrow \mathbb{R}^{3 \times 3}$ is now taken to be, in the (ξ, η, ζ) -frame,

$$\beta(\xi, \eta, \zeta) \in \left\{ \begin{pmatrix} 0 \\ s_2 \\ s_3 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} s_1 \\ 0 \\ s_3 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} s_1 \\ s_2 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}, \quad (53)$$

for a.e. $(\xi, \eta, \zeta) \in \Omega_L$, and there is no restriction on the $s_i(\xi, \eta, \zeta)$. Note that this is a somewhat weaker condition than the one in (2), in the sense that we allow any Burgers vector which lies within a given slip plane, and not just those in the direction of the cubic-lattice-face diagonals. Of course, any lower energy bound for the relaxed condition still holds for the original one.

In this setting, for a.e. (ξ, η, ζ) , we have

$$\beta = \begin{pmatrix} 0 & \beta_{\xi\eta} & \beta_{\xi\zeta} \\ \beta_{\eta\xi} & 0 & \beta_{\eta\zeta} \\ \beta_{\zeta\xi} & \beta_{\zeta\eta} & 0 \end{pmatrix}, \quad (54)$$

and for a.e. slice of constant ζ (call it S_ζ), the 2-d side condition holds: $\beta_{\xi\eta} = 0$ or $\beta_{\eta\xi} = 0$ for a.e. $(\xi, \eta) \in S_\zeta$.

Now, consider the energy functional (1), with τ set to zero and subject to the relaxed side condition (53). Denote by $(\nabla u - \beta)_{\text{sym}}^{2 \times 2}$ the (ξ, η) -components of the elastic strain, and, for fixed ζ , define the reduced slice energy, E_L^ζ , by

$$E_L^\zeta(u, \beta) = \iint_{S_\zeta} \left| (\nabla u - \beta)_{\text{sym}}^{2 \times 2} \right|^2 + |\partial_\xi \beta_{\xi\eta}| + |\partial_\eta \beta_{\eta\xi}| \, d\xi d\eta. \quad (55)$$

Then, clearly, $E_L(u, \beta) \geq \int_0^1 E_L^\zeta \, d\zeta$, and, since all of our 2-d lower bounds from previous sections apply to E_L^ζ , for a.e. ζ , they also go through for the B2 crystal oriented as above. Meanwhile, the upper bounds for the energy can be recovered in the following way. First, simply take the same test function, (u, β) , as for the 2-d case, extend constantly in the ζ direction, and let $\beta_\zeta = \beta_{,\zeta} = 0$. This establishes the upper bounds subject to the relaxed side condition (53). The original side condition can be recovered by introducing fine oscillations between the two possible Burgers vectors, in the active slip planes along the slip-plane normal. Note that such a microstructure is a gradient field even without the introduction of a lattice rotation[§], and thus does not make any contribution to the curl term.

In summary, we have proved

Theorem 3.1. *The upper and lower bounds of Theorems 2.8-2.12 also hold for the energy (1) with $\tau = 0$, subject to (52), as applied to a B2 crystal occupying the domain $\Omega_L = (0, 1) \times (0, L) \times (0, 1)$ with slip-plane normals oriented as above, and such that the cross-hardening condition (53) is satisfied.*

Remark 3.2. For the case of a non-zero, constant strain hardening, i.e. $\tau > 0$, the energy scaling is as follows. For $L \geq 2$, the minimal energy is now at most $\tau\gamma$, which is easy to see by inspecting the 2-d test function used previously. For $L < 1$, we still have the same quadratic scaling of the energy with respect to (large) γ as before, since the upper-bound test function of Figure 9 gives a strain-hardening energy of order $\tau\gamma$. In the regime $1 \leq L < 2$, the linear scaling of the energy with respect to γ is preserved: the proof for the lower bound goes through unchanged, while inspection of the test function for the upper bound yields an additional contribution to the energy of order $\tau\gamma$. Furthermore, for a physically realistic model, we would expect τ to be small compared to both the elastic modulus (implicitly equal to unity here) and σ . This is due to the fact that the L^1 -penalty on β only accounts for self-hardening, i.e. the hardening which occurs if the specimen is deformed purely in single slip—all other hardening is taken care of by the single-slip side condition and the surface energy.

4 The scalar model

In this section, we take a brief (and salutary) look at an ostensibly simplified scalar version of the model (3)-(5) which is analogous to that treated in section 4 of [12]. Rather than imposing a soft Dirichlet condition on the whole of $\partial\overline{\Omega}_L$ as in [12], however, we continue to use a hard Dirichlet condition to model a fixed horizontal shear imposed by clamping both ends of the single-crystal specimen.

[§]It is in fact a rotated version of $\begin{pmatrix} 0 & \beta_{12}(x_2) & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ in x_i -coordinates. Note that the row-wise curl of such a matrix vanishes identically, independently of the scalar function $\beta_{12}(x_2)$.

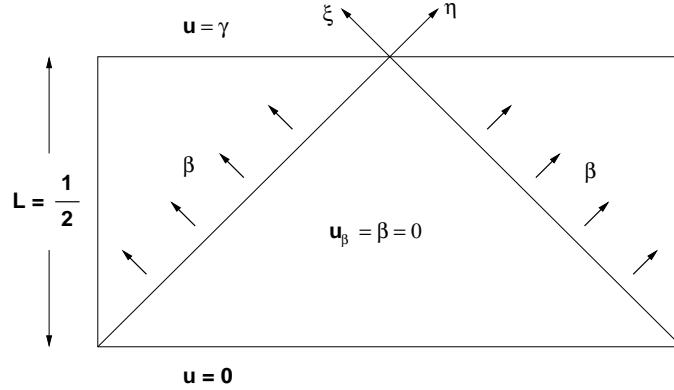


Figure 16: Test functions used in the proof of Theorem 4.1.

As before, the rectangular specimen occupies the domain $\overline{\Omega}_L = (0, 1) \times (0, L) \subset \mathbb{R}^2$, but this time we focus attention on just the x_1 -component of the deformation field, denoted by $u: \overline{\Omega}_L \rightarrow \mathbb{R}$, and the plastic strain, $\beta: \overline{\Omega}_L \rightarrow \mathbb{R}^2$, which are to be obtained by minimising the functional

$$E_L^s(u, \beta) = \int_{\overline{\Omega}_L} |\nabla u - \beta|^2 dx + \int_{\overline{\Omega}_L} |\nabla \times \beta|, \quad (56)$$

subject to the side condition $\beta_1 = \pm\beta_2$, in the sense of distributions in $\overline{\Omega}_L$, and where the second term in (56) is the measure-theoretic quantity defined in [12]. This quantity can be obtained from (5) by making the substitutions $\beta_{\xi\eta} \rightarrow \beta_\eta$ and $\beta_{\eta\xi} \rightarrow \beta_\xi$ in the usual rotated (ξ, η) co-ordinates. In these co-ordinates, the side condition on β takes the form: $\beta_\xi = 0$ or $\beta_\eta = 0$ for a.e. $(\xi, \eta) \in \overline{\Omega}_L$.

We prescribe free boundary conditions on the two ‘vertical’ sides of $\overline{\Omega}_L$, and a fixed average shear, γ , in the x_1 direction on the remaining two sides. In other words, $\langle n, \nabla u - \beta \rangle = 0$ on $\partial\overline{\Omega}_L \cap \{x_1 = 0, 1\}$, where n is the unit normal to $\partial\overline{\Omega}_L$, $u = 0$ on $\partial\overline{\Omega}_L \cap \{x_2 = 0\}$ and $u = \gamma$ on $\partial\overline{\Omega}_L \cap \{x_2 = L\}$.

Now we write $J_L^s = \inf E_L^s(\cdot, \cdot)$, and ask how J_L^s varies with the L . It turns out that analysing this question is no easier than in the full vector-valued case, and that, in fact, there is a qualitative difference between the results for the scalar model and those for the vector-valued model subject to either **BC1** or **BC2**.

First of all we note that J_L^s is left-continuous and monotonically decreasing, by the same arguments used in Propositions 2.1 and 2.2. Then the next Theorem, combined with the foregoing remark, implies that $J_L^s = 0$ for $L \geq \frac{1}{2}$ and that there is no jump in the energy at $L = \frac{1}{2}$: the difference between this result and those for **BC1** and **BC2** is explained by the fact that there is no constraint on the vertical deformation in the scalar model, which is rather unphysical. Whether the energy is strictly positive for $L < \frac{1}{2}$ remains an open question.

Theorem 4.1. *Subject to $u = 0$ at $x_2 = 0$ and $u = \gamma$ at $x_2 = \frac{1}{2}$, we have $J_{\frac{1}{2}}^s = 0$.*

Proof. Let $L = \frac{1}{2}$, and centre the (ξ, η) co-ordinates at the mid-point of the top boundary, as shown in Figure 16.

Now, for each $\alpha \in (0, 1)$, construct test functions (u_β, β) by setting $u_\beta = \beta = 0$ on $\{\xi > 0, \eta < 0\}$,

$$u_\beta = \gamma(2\sqrt{2}\xi)^\alpha, \quad \beta = \nabla u_\beta \quad \text{on} \quad \{\xi > 0, \eta < 0\}, \quad (57)$$

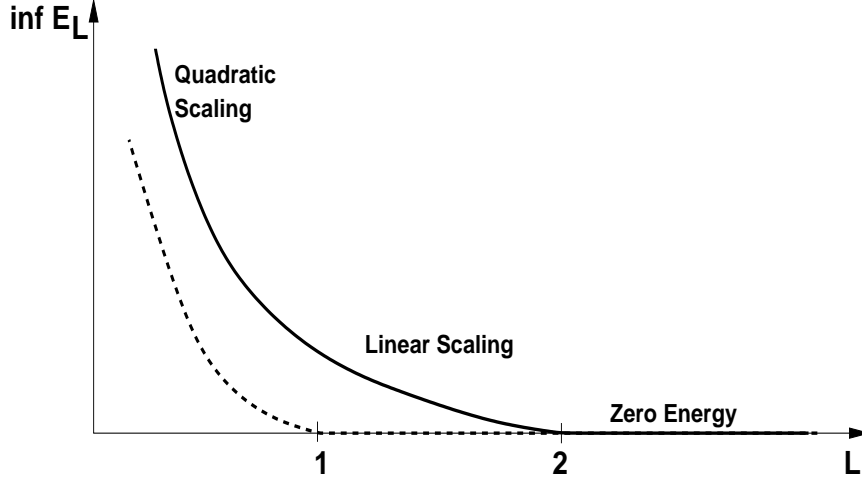


Figure 17: Schematic of the different scaling regimes for the energy (1) with $\tau = 0$. The solid line represents the energy when both $\sigma > 0$ and the single-slip condition is enforced—in this case, the energy vanishes for $L \geq 2$, scales linearly with the (large) applied strain γ for $1 \leq L < 2$, and scales quadratically for $L < 1$. The dashed line shows the energy when either $\sigma = 0$ or the single-slip side condition is dropped. In this case, the linear energy-scaling regime is no longer present.

and

$$u_\beta = \gamma(2\sqrt{2}\eta)^\alpha, \quad \beta = \nabla u_\beta \quad \text{on} \quad \{\xi < 0, \eta > 0\}. \quad (58)$$

Thus, $\nabla \times \beta = 0$, and, in the now familiar way, we write $v = u - u_\beta$, where u is the unknown deformation, and we look for v which minimises $\|\nabla v\|_{L^2}^2$, subject to the Dirichlet conditions

$$v = \begin{cases} 0 & : x_2 = 0 \\ \gamma(1 - (2\sqrt{2}\xi)^\alpha) & : x_2 = \frac{1}{2}, \eta < 0 \\ \gamma(1 - (2\sqrt{2}\eta)^\alpha) & : x_2 = \frac{1}{2}, \xi < 0 \end{cases} \quad (59)$$

The fact that $\|\nabla v\|_{L^2}$ can be made arbitrarily small as $\alpha \rightarrow 0$ follows by analogy with the proof of Theorem 2.5, given the shape of the Dirichlet data. \square

5 Conclusions

We have derived energy-scaling results and explicit bounds for the elasto-plastic energy in a realistic single-crystal shear experiment. The different scaling regimes under various assumptions are summarised in Figure 17. As discussed in the introduction, the results obtained should provide a means of discriminating between two different classes of models in crystal plasticity: those with strong cross-hardening and surface energy, and those without. It is, however, open as to whether our results carry over from the B2 case to more common crystal structures, such as face-centred-cubic or hexagonal-close-packed lattices.

Of course, in this article, we have only considered a geometrically linear elasto-plastic energy, and while our upper bounds should still hold in the geometrically nonlinear case, using a multiplicative decomposition of the strain, obtaining the lower energy bounds is a much more challenging problem,

and is the subject of ongoing work. A further objective is to carry out numerical simulations of the deformation predicted by our modelling.

Finally, the experiments themselves are also work in progress, and will be performed in collaboration with the Max Planck Institut für Eisenforschung in Düsseldorf—one of the main practical problems in this regard will be to impose the boundary conditions without slippage or other spurious deformation.

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